Optimizing the FDFD Method in Order to Minimize PML-Related Numerical Problems

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Abstract **— Using the PML boundary condition in the finite-difference frequency-domain (FDFD) method can significantly affect the numerical condition of the resulting system of equations, causing a drastic increase in the CPU time. This paper presents in-depth investigations of the underlying effects as well as measures to improve numerical convergence. The results are verified for various microwave structures such as a flip-chip interconnect, a multi-layer transition, and a patch antenna. They apply not only to the FDFD method but similarly to other frequency-domain as well as time-domain approaches.**

Index Terms **— PML, finite-difference, Convergence.**

I. Introduction

Today electromagnetic simulation represents an indispensable tool in the development of microwave and mm-wave circuits and modules. Its capabilities have been extended significantly during the last decade, partly due to the advances in computer hardware, partly due to improvements in numerical mathematics.

Beyond this, the Perfectly Matched Layer (PML) concept has greatly contributed to that success. Description of the boundary of the computational domain has always been a key issue in bringing up efficiency of electromagnetic (EM) simulation, and PML provides an excellent solution to this issue. It was introduced by Berenger [2] and is based on the splitting of Cartesian electric and magnetic field components into two subcomponents. Alternatively, it can be realized by introducing anisotropic material properties, with electric and magnetic conductivities, leading to permeability and permittivity tensors [3].

Today, PML forms a salient feature of all common 3D EM simulation methods, both in the time domain (FDTD, TLM) and the frequency domain (finite-element method, FDFD). In the latter case, mostly the anisotropic material approach [3] is applied because it can be easily implemented without any need to modify the Maxwell's equations.

However, the benefits of PML do not come for free. In the frequency-domain case, the material tensors worsen the numerical properties of the system of equations to be solved, which results in increased CPU time. In the time domain, mechanisms are not such clearly to be identified but similar effects are observed. Generally, the deteriorations depend strongly on the number and parameters of the PML layers and occur particularly if PLM layers overlap, e.g., at the edges and corners of the outer boundary of the computational domain.

While numerous papers have been published on the advantages of the PML, the PML-related difficulties are less present in the literature. In fact, the authors are not aware of any publication addressing convergence problems due to PML, neither in frequency-domain nor in time-domain descriptions. This is presented here together with recommendations how to circumvent or alleviate these difficulties.

The following treatment is based on the finite-difference method in frequency domain (FDFD) with the PML implemented according to the anisotropic material approach [3] as described in [5]. After a description of the PML formulation and basic considerations in Sec. II, several critical issues and the respective measures to minimize numerical efforts are discussed, i.e., how to handle overlapping PML layers in edges and corners (Sec. III), and how to choose PML cell size properly (Sec. IV), which turned out to be a key factor.

II. Basic Considerations

Our FDFD formulation is described in [1,5,6]. Basically, as in all finite-element and finite-difference frequency-domain approaches, the original problem is reduced to a boundary-value problem, i.e., a large system of linear equations has to be solved, with the unknowns being the field values on the mesh. With PML, the system matrix is complex-valued, also if a lossless structure is simulated. This system is solved employing iterative numerical algorithms; in our case they are of the SSOR type. Changing the numerical properties of the system matrix, as done when introducing PML layers, for instance, affects convergence of the solver, i.e., the number of iterations. This number is taken here as a measure for the numerical efforts. It is directly proportional to the CPU time needed to obtain the solution.

Regarding the PML, some further details should be mentioned here for the sake of completeness:

- As well known (e.g. [4]), in a discretized description the interface of the PML/non-PML regions results in spurious reflections. This mismatch problem can be alleviated by subdividing the PML region into a number of layers with varying conductivity [2]. This

approach is applied throughout this paper (for details see [6]).

- The number of PML layers plays an important role, of course. More layers improve accuracy but increase numerical expenses. We found that a 5-layer configuration provides a good compromise and this number is used in all following investigations.
- The convergence of the iterative solver is influenced also by the choice of the PML backing. Commonly, PML walls are followed by electric or magnetic walls. We found that electric walls lead to less iterations than magnetic walls.

When discussing the numerical consequences of introducing PML, it is important to have a close look on the resulting permittivity and permeability tensors, which are written here as products of the isotropic physical material constants multiplied with a tensor [η] representing the PML properties according to [3, 4] (see eqns. (1) and (2)).

$$[\overline{\boldsymbol{\varepsilon}}] = \varepsilon_0 \varepsilon_r [\overline{\boldsymbol{\eta}}] \tag{1}$$

$$[\overline{\boldsymbol{\mu}}] = \mu_0 \mu_r [\overline{\boldsymbol{\eta}}] \tag{2}$$

[η] is a diagonal tensor with the complex parameter η_i defining the attenuation and thus the residual reflections at the PML (see Fig. 1). Low reflection, i.e., high attenuation in the PML, means that the imaginary part of η_i dominates assuming magnitudes much larger than unity.

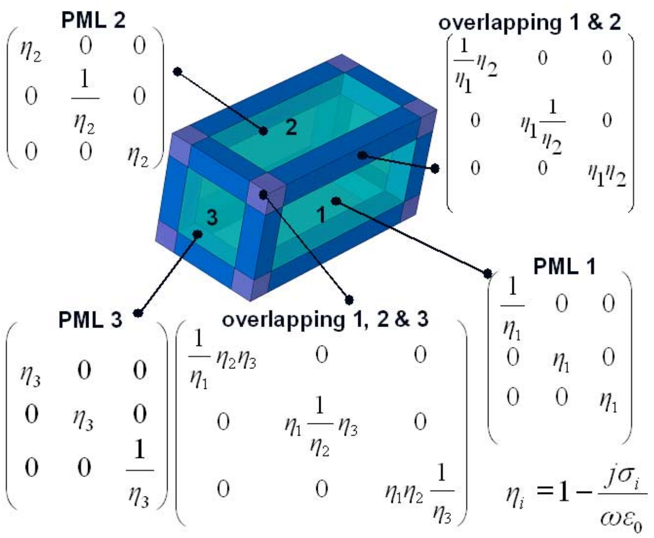

Fig. 1 : PML Tensors [η] (see (1) and (2)) for PML walls in three directions detailing the overlapping regions. σ_i denotes the artificial conductivities of the respective PML wall as derived from a given nominal reflection factor.

When using PML walls for several outer boundaries, these walls overlap at edges and corners as illustrated by Fig. 1. In case of overlapping at edges (e.g. overlapping 1 & 2) and corners (overlapping 1, 2 & 3) the resulting PML tensor is the product of the PML tensors of the individual PML walls that form the edges and corners, respectively.

Inspection of the tensors according to Fig. 1 reveals that, because always both η_i and its inverse appear, the PML increases the magnitude range of the material tensors and thus that of the resulting entries in the system matrix, which in turn increases the radii of the well known Gerschgorin circles. These circles contain all the eigenvalues of the system matrix and larger radii of those circles means higher possibilities of the real parts of the eigenvalues to be more negative and thereby worse convergence. This situation becomes particularly critical for the overlapping regions since there several factors η_i are multiplied. In order to demonstrate this, Tab. 1 shows typical values for the PML tensor elements (based on an example at 1GHz with –60dB nominal reflection). This is the basic effect why PML causes the numerical properties to deteriorate but one needs an in-depth investigation to better understand the underlying effects and to find solutions minimizing the odds. This is presented in the following Sections III and IV.

$\lvert\eta_1\rvert$	$\lvert 1/\eta_1\rvert$	$\lvert\eta_2\rvert$	$\lvert 1/\eta_2\rvert$
83.0	0.012	75.0	0.013
$\lvert(1/\eta_1)\eta_2\rvert$	$\lvert\eta_1\eta_2\rvert$	$\lvert(1/\eta_1)\eta_2\eta_3\rvert$	$\lvert\eta_1(1/\eta_2)\,\eta_3\rvert$
0.9	6225	67.5	83

Tab. 1 Diagonal elements of PML tensors according to Fig. 1 (ε_r of PML wall 1 and 2 are 1.0 and 2.2 respectively; σ_i of PML wall 1 and 2 are 4.6 and 4.2 respectively; μ_r is 1.0 in all cases; for calculation of σ_i see [4, 6]).

III. Overlapping PMLs

While for a single PML wall the tensor elements are in the range $1/\eta$ … 1 … η, this becomes worse if overlapping regions of two PML walls are included. Assuming that both PML walls have the same properties, the tensor elements within the structure now cover the range $1/\eta$ … 1 … η^2. Proceeding with 3 overlapping PML regions the overall situation does not change from this point of view because the additional elements are of same order (if one assumes identical PML properties).

Going beyond these relatively simple arguments, we performed extensive investigations simulating typical microwave structures with different PML configurations. We found that the PML disposition indeed has a drastic influence on the efforts required for solving the system of equations. Introducing a single PML wall already leads to a significant increase in the number of iterations of the solver (typically a factor of 2). Including overlapping regions with 2 PML results in further drastic deteriorations (an additional factor >15), which in many cases render this approach useless for practical design work.

We tried to alleviate this situation by modifying the PML definition in the edge and corner regions. Different ideas have been tested including an angle-dependent description and the insertion of additional physical conductivities in the PML formulation for numerical stabilization. All these approaches did not yield the desired improvements. The best solution turned out to be to avoid any overlapping. Since edges and corners form only a very small fraction of the overall PML surface, reflections occurring there remain negligible in almost any case and one can use a PML with attenuation in a single direction instead. Fig. 2 illustrates this for the edge case.

This approach to circumvent the problem with overlapping PMLs has proven its effectiveness for various structures like patch antenna, microstrip, flip-chip or LTCC structures. For example, simulating a patch antenna (see Fig. 6) with PML fully including the overlapping descriptions results in an iteration count above 300,000 (above 3 GHz), while with non-overlapping PML walls the number of iterations can be kept below 7,000. One should note that the choice of PML direction in the edge and corner regions termed as orientation in Fig. 2 affects convergence. One of the reasons is the construction of the system matrix where the order of elements influences the number of iterations.

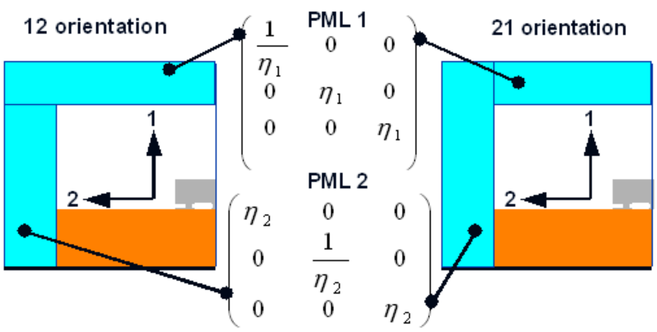

Fig. 2: Edge of the structure according to Fig. 1 with non-overlapping PML walls (2 possibilities) .

IV. PML Cell Size

One parameter unexpectedly turned out to be a vital quantity, which greatly affects numerical convergence. This is the cell size within the PML layers. Extensive investigations have been carried out in order to check the influence of PML cell size on accuracy and numerical convergence.

As an example, Fig. 3 shows a microstrip structure with a PML followed by an electric wall at the end of the structure, which was simulated applying different cell sizes and a fixed nominal reflection factor of -60 dB. Fig. 4 illustrates the cell sizes in longitudinal direction for three different discretization schemes. The cross-sectional discretization remains the same for all these three cases, and the largest cell size in lateral direction is below 40 µm. The resulting number of iterations (and hence the CPU time) is plotted in Fig. 5. Clearly, the best results over the entire frequency range are obtained if the PML cells are larger than the non-PML cells.

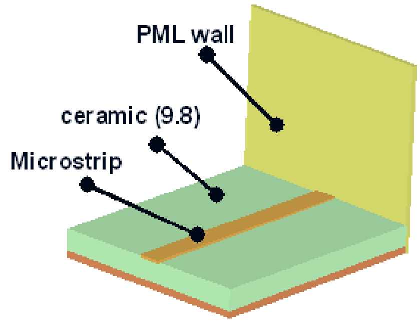

Fig. 3: Microstrip structure with PML wall placed at the end in longitudinal direction.

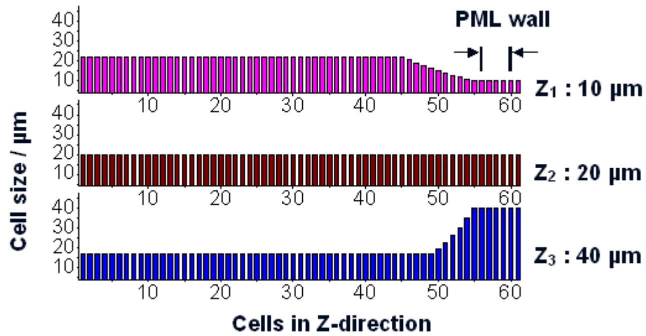

Fig. 4 Discretizations used for the microstrip of Fig. 3. For version z_1 (top), PML cells are the smallest ones; for version z_2, the mesh is homogeneous, for z_3 (bottom), PML cells are the largest ones (Z_3).

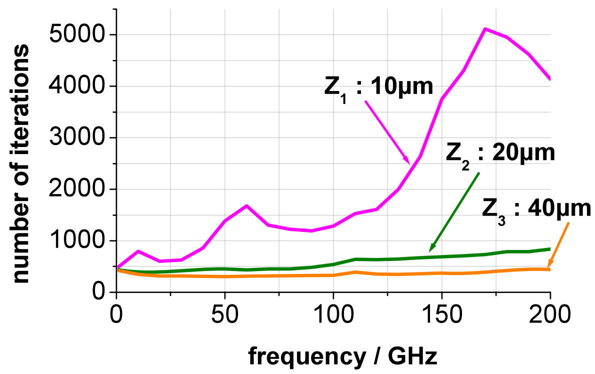

Fig. 5: Iterations for the different discretization schemes according to Fig. 4 as a function of frequency (microstrip structure of Fig. 3).

The microstrip structure of Fig. 3 is a too simple example to draw general conclusions, of course. Therefore, we checked our findings for various microwave structures, like flip-chip

interconnects, a patch antenna, and a spiral inductor. In all cases, choosing PML cells to be the largest improved convergence thus supporting the results in Fig. 5.

It should be stressed that cell size in the PML should be the largest within the structure but there is no necessity to choose it much larger. Increasing PML cell size further and further the reduction in number of iterations reaches a saturation. Of course, PML cell size must be smaller than about one tenth of the wavelength in order to keep dispersion error low.

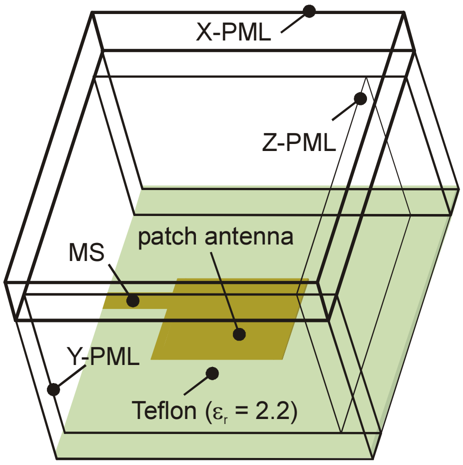

Fig. 6: Patch antenna (see [4]) with PML walls placed in positive x, y and z and negative y directions.

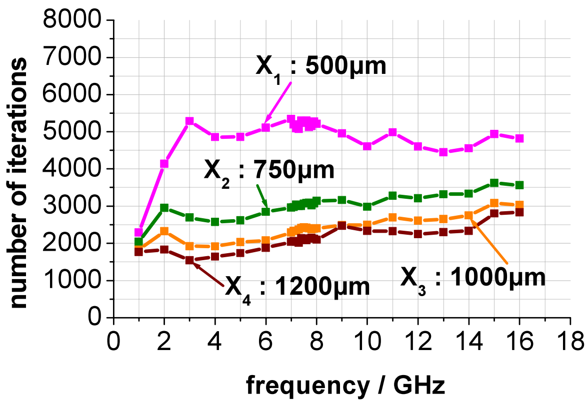

Fig. 7: Structure of Fog. 6: Number of iterations for different x discretizations; PML cell sizes in y and z directions are 900 µm (with non-PML cell sizes all below 900 µm).

Finally, in order to demonstrate the effect of PML cell size for a radiating structure, the patch antenna according to Fig. 6 was simulated with different PML wall configurations in all open directions. The PML walls are non-overlapping following the approach of Sec. II, with the following orientation: The x-directed PML overrides all other PMLs, the y-directed ones override the z-directed one. Accordingly, this is termed as x-y-z orientation. The x PML cell sizes vary from 500 to 1200 µm and the y and z PML cells from 500 to 900 µm. The corresponding numbers of iterations are plotted in Fig. 7.

The results of Fig. 7 support the observations made before: PML cell size should be chosen equal to or larger than that of the remaining mesh cells, which in this case is 900µm. For a cell size of 1000 µm, one obtains about half the number of iterations than for 500 µm, which is a really significant change, increasing PML cell size further yields only slight improvements.

V. Conclusions

Using PML as absorbing boundary condition has become the method of choice due to its superior low-reflective properties. However, the artificial PML material changes the numerical properties of the simulation problem, in frequency-domain formulations this shows up in the matrix of the resulting system of equations and the related numerical efforts. For the finite-difference frequency-domain method (FDFD), the following guidelines are found to be effective in optimizing the performance in the presence of PML layers:

- Use only non-overlapping PML walls
- Choose cell sizes within the PML equal to or larger than the non-PML cell sizes in all directions.

These results were obtained for the FDFD method but the PML-related consequences should apply to other frequency-domain formulations (e.g., FE method) as well and, in an analog way, also to time-domain schemes such as FDTD.

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